

Application No. 09/696,071

RD-28030

## AMENDMENTS TO THE CLAIMS:

This listing of claims will replace all prior versions and listings of claims in the application:

**Listing of Claims**

1. (currently amended) A method, comprising:

(A) defining a first experimental space comprising factors of at least two mixtures with at least one common factor;

(B) determining a number of experiments for a succeeding second experimental space by the relationship

$$V + \prod_{i=1}^3 n_i \times L_3 + \left[ \sum_{i=1}^3 \frac{1}{n_i} \prod_{j=1}^{i-1} n_j \right] \times L_2 ;$$

for a ternary system ( $T=3$ ) or an algorithm for a succeeding  $T$ -nary system, determined from a previous term by:(a) adding an additional term which contains an additional summation, incremented over a next index from a starting point one unit higher than the first summation; (b) decrementing the subscript on  $L$ ; and (c) adding a value of  $n$ , indexed by the next index, to the inverse term;

(C) deleting duplicate factor combinations from the first determined experimental space to define a succeeding second experimental space with a number of experiments determined in (B); and

(D) conducting a combinatorial high throughput screening (CHTS) experiment on said succeeding second experimental space, comprising an iteration of steps of simultaneously reacting a multiplicity of tagged reactants and identifying a multiplicity of tagged products of the reaction and evaluating said identified products after

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completion of a single or repeated iteration to select a best case set of factors from said second experimental space.

2. (canceled)

3. (canceled)

4. (canceled)

5. (canceled)

6. (canceled)

7. (currently amended) The method of claim 1, wherein said succeeding second experimental space factors comprise reactants, catalysts and conditions and said (D) comprises (a) reacting a reactant selected from the succeeding second experimental space under a set of catalysts or reaction conditions selected from the succeeding second experimental space and (b) evaluating a set of products of the reacting step and further comprising (E) reiterating step (D) wherein a next succeeding second experimental space selected for a step (a) is chosen as a result of an evaluating step (b) of a preceding iteration of step (D).

8. (previously presented) The method of claim 7, comprising reiterating (D) until a best set of factors of said second experimental space is selected.

9. (original) The method of claim 1, wherein said first experimental space includes a catalyst system comprising combinations of Group IVB, Group VIB and Lanthanide Group metal complexes.

10. (currently amended) The method of claim 1, wherein said succeeding second experimental space includes a catalyst system comprising a Group VIII B metal.

11. (currently amended) The method of claim 1, wherein said succeeding second experimental space includes a catalyst system comprising palladium.

12. (currently amended) The method of claim 1, wherein said succeeding

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second space includes a catalyst system comprising a halide composition.

13. (currently amended) The method of claim 1, wherein said succeeding second experimental space includes an inorganic co-catalyst.

14. (currently amended) The method of claim 1, wherein said succeeding second experimental space includes a catalyst system that includes a combination of inorganic co-catalysts.

15. (canceled)

16. (canceled)

17. (canceled)

18. (currently amended) A system for selecting a best case set of experiments of a experimental reaction, comprising;

a processor that (A) defines a first experimental space comprising factors of at least two mixtures with at least one common factor; (B) determines a number of experiments for a succeeding second experimental space by the relationship

$$V + \prod_{i=1}^3 n_i \times I_3 + \left[ \sum_{i=1}^3 \frac{1}{n_i} \prod_{j=1}^{i-1} n_j \right] \times I_2$$

for a ternary system ( $T = 3$ ) or an algorithm for a succeeding  $T$ -nary system, determined from a previous term by:(a) adding an additional term which contains an additional summation, incremented over a next index from a starting point one unit higher than the first summation; (b) decrementing the subscript on  $I$ ; and (c) adding a value of  $n$ , indexed by the next index, to the inverse term; and (C) deletes duplicate factor combinations from the first determined experimental space to define a succeeding second experimental space with a number of experiments determined in (B); and

a reactor and evaluator to select a best case set of factors from said succeeding second experimental space by a combinatorial high throughput screening (CHTS) method

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to select a best case set of factors from said experimental space.

19. (original) The system of claim 18, wherein said processor comprises

a display terminal having screen displays whereby a researcher can input values for factors on said screen;

a database for storing said factors;

a computer for generating a set of test cases for a set of said factors based on a researcher specified value for identifying a number of interacting relationships within said factors;

a computer combining said test cases for set of factors with said relationships and providing a merged table of test cases; and

an output for writing to a database said merged table of test cases.

20. (canceled)

21. (currently amended) The system of claim 18, wherein said succeeding second experimental space is a quaternary space comprising a number of experiments defined by

$$V + \prod_{i=1}^4 n_i \times I_4 + \left[ \sum_{i=1}^4 \frac{1}{n_i} \prod_{i=1}^4 n_i \right] \times I_3 + \left[ \sum_{i=1}^4 \sum_{j=i+1}^4 \frac{1}{n_i n_j} \prod_{i=1}^4 n_i \right] \times I_2$$

22. (currently amended) The system of claim 18, wherein said succeeding second experimental space is a pentenary space comprising a number of experiments defined by

$$V + \prod_{i=1}^5 n_i \times I_5 + \left[ \sum_{i=1}^5 \frac{1}{n_i} \prod_{i=1}^5 n_i \right] \times I_4 + \\ \left[ \sum_{i=1}^5 \sum_{j=i+1}^5 \frac{1}{n_i n_j} \prod_{i=1}^5 n_i \right] \times I_3 + \left[ \sum_{i=1}^5 \sum_{j=i+1}^5 \sum_{k=j+1}^5 \frac{1}{n_i n_j n_k} \prod_{i=1}^5 n_i \right] \times I_2 .$$

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23. (original) An experimental space, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{i=1}^T n_i \times I_T + \left( \sum_{i=1}^T \frac{1}{n_i} \right) \times \left( \prod_{i=1}^T n_i \right) \times [I_{(T-1)}]$$

for a ternary system ( $T = 3$ ) or an algorithm for a succeeding  $T$ -nary system, determined from a previous term by: (a) adding an additional term which contains an additional summation, incremented over a next index from a starting point one unit higher than the first summation; (b) decrementing the subscript on  $I$ ; and (c) adding a value of  $n$ , indexed by the next index, to the inverse term.

24. (original) The experimental space of claim 23, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{i=1}^4 n_i \times I_4 + \left[ \sum_{i=1}^4 \frac{1}{n_i} \prod_{i=1}^4 n_i \right] \times I_3 + \left[ \sum_{i=1}^4 \sum_{j=i+1}^4 \frac{1}{n_i n_j} \prod_{i=1}^4 n_i \right] \times I_2$$

for a quaternary system.

25. (original) The experimental space of claim 23, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{i=1}^5 n_i \times I_5 + \left[ \sum_{i=1}^5 \frac{1}{n_i} \prod_{i=1}^5 n_i \right] \times I_4 + \\ \left[ \sum_{i=1}^5 \sum_{j=i+1}^5 \frac{1}{n_i n_j} \prod_{i=1}^5 n_i \right] \times I_3 + \left[ \sum_{i=1}^5 \sum_{j=i+1}^5 \sum_{k=j+1}^5 \frac{1}{n_i n_j n_k} \prod_{i=1}^5 n_i \right] \times I_2$$

for a pentanary system.